

ORBITAL MAGNETISM IN THE CUPRATES

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The pseudogap phase of the cuprate superconductors is argued to be characterized by a hidden broken symmetry of d -wave character in the particle-hole channel that leads to staggered orbital magnetism. This proposal has many striking phenomenological consequences, but the most direct signature of this order should be visible in the neutron scattering experiments. The theoretical underpinning of these experiments is discussed.

1 Introduction

It has been proposed that the pseudogap state is a phase with a broken symmetry and an order parameter,^{1,2} not a state with a merely fluctuating order.³ The distinction between the two is enormous. The order parameter, which is due to a particle-hole condensate with internal “angular momentum” 2, will be termed the d -density wave (DDW). We have predicted that the present day neutron scattering experiments have enough resolution to provide a direct evidence of this order. And, indeed, there are some preliminary neutron scattering measurements in the bilayer $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ that appear to have observed the theoretically predicted order parameter.^{4,5} There are other experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{6.5}$, which observe a magnetic signal,⁶ but appear to be from remnant spins left over from the undoped antiferromagnet. While the experimental situation must be resolved, we shall focus merely on the theoretical predictions because a precise analysis is necessary to make sure that what is being observed is not an artefact. The fundamental signature of this order parameter is an elastic Bragg peak centered at two-dimensional wave vector $\mathbf{Q} = (\pi/a, \pi/a)$, where a is the lattice spacing of the CuO-lattice. Since the magnitude of the staggered orbital fields is of order 10 G, the experiments are difficult.

The neutron scattering from DDW was addressed previously,⁷ but the polarized neutron scattering and the important question about the current form factors were not. The current form factors play an important role in polarized neutron measurements, without them one may be led to physically incorrect results. Moreover, the crucial connection to the pseudogap phase was not made, nor was it made clear that such a phase truly survived beyond the

large- N mean field theory due to presumed gauge fluctuations. There is also a proposal⁸ of a circulating current phase, which does not break translational symmetry. The similarity with the DDW state is merely superficial. At the very least, the signature, on robust symmetry grounds, is a neutron signal at $Q = 0$ which is fundamentally different. We will have nothing to say about this proposal, as it is not germane to the present set of experiments.

2 Order parameter

The singlet DDW is defined by the order parameter $\Phi_{\mathbf{Q}}$ in terms of a particle-hole condensate⁹

$$\langle c^{\sigma\dagger}(\mathbf{k} + \mathbf{Q}, t) c_{\rho}(\mathbf{k}, t) \rangle = i \frac{\Phi_{\mathbf{Q}}}{2} (\cos k_x a - \cos k_y a) \delta_{\rho}^{\sigma}, \quad (1)$$

where σ, ρ are spin indices. The order parameter breaks time reversal, parity, translation by a lattice spacing, and the rotation by $\pi/2$, although the product of any two of these is preserved. Interestingly, DDW does not modulate charge at all, but it modulates currents. The reason it is still called a density wave is because it is a particle-hole condensate, and d -wave refers to the internal form factor of the particle and the hole, which is $(\cos k_x a - \cos k_y a)$. We expect that the magnetic field generated by the circulating currents should be proportional to the pseudogap.² A simple estimate results in a tiny field of order 10 G due to currents circulating in a CuO plaquette as shown below:

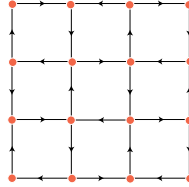


Figure 1. Circulating current pattern in the model where the current is carried by δ -function wires.

Although this simple model captures the correct symmetry, it is crucially deficient in predicting the correct neutron scattering intensities, as we shall see. It is *a priori* clear that the flow of currents cannot be along infinitesimally thin wires, but it must spread out, both because of finite sized atomic orbitals and because of electron-electron interactions. One can model the more realistic current distribution⁵ by the form factors $\alpha(\mathbf{q})$ and $\beta(\mathbf{q})$ in the Fourier

transform of the current distribution $\langle \mathbf{j}(\mathbf{q}) \rangle$ without destroying the symmetry of the order parameter ($\mathbf{q} \cdot \langle \mathbf{j}(\mathbf{q}) \rangle = 0$), where

$$\begin{aligned} \langle \mathbf{j}(\mathbf{q}) \rangle &\propto \Phi_{\mathbf{Q}} \sum_{\mathbf{G}_{\parallel}} \delta_{\mathbf{q}_{\parallel}, \mathbf{G}_{\parallel}} f(\mathbf{q}) \\ &\times \left[\left(\alpha(\mathbf{q}) \frac{\hat{\mathbf{x}}}{q_x} - \beta(\mathbf{q}) \frac{\hat{\mathbf{y}}}{q_y} \right) - (\alpha(\mathbf{q}) - \beta(\mathbf{q})) \frac{\hat{\mathbf{z}}}{q_z} \right]. \end{aligned} \quad (2)$$

Here, $\mathbf{q}_{\parallel} = (q_x, q_y)$, $f(\mathbf{q}) = \sin(\frac{q_z d}{2})$, d is the separation between the two CuO-planes within a bilayer complex, and \mathbf{G} is a reciprocal lattice vector. The simplest choice is to take $\alpha(\mathbf{q})$ and $\beta(\mathbf{q})$ to be dependent on q_z only, such that $\alpha(q_z) - \beta(q_z) \sim q_z^2$, as $q_z \rightarrow 0$. The choice of this current density was discussed in Ref. 5.

3 Experimental detection of DDW

The DDW is usually hard to detect because

$$\sum_{\mathbf{k}} \langle c^{\sigma\dagger}(\mathbf{k} + \mathbf{Q}) c_{\rho}(\mathbf{k}) \rangle \propto \sum_{\mathbf{k}} (\cos k_x a - \cos k_y a) = 0 \quad (3)$$

There is no net modulation of charge and spin that could be measured. Contrast this with a d -wave superconductors (DSC) for which a similar momentum sum of the particle-particle condensate also vanishes. Nonetheless, because of broken gauge symmetry, Meissner effect follows, irrespective of the pairing channel. This is not possible for a DDW because the broken symmetry is in the Ising universality class, and experiments seeking to uncover such order must (a) be sensitive to spatial variation of kinetic energy or currents, (b) measure higher order correlations of the charge or spin density as in 2-magnon Raman scalletring, nuclear quadrupole resonance, etc.⁹ One nice feature of DDW is that a thermodynamic transition is possible in two dimensions due to the Ising nature of the order parameter.

Impurities will mix d -wave order with the s -wave order proportional to the concentration of impurities. This may be an indirect way to reveal the hidden broken symmetry, because the corresponding s -wave order is none other than the conventional charge density wave (CDW). Another possibility is spin-orbit coupling, which will mix spin density wave (SDW) with DDW. In mean field theory,¹⁰ there is some evidence that DDW may incommensurate for higher doping. If this is the case, the charge order must inevitably be mixed in, an idea that can be experimentally probed by scanning tunneling measurements inside the vortex core of the mixed DDW and DSC phase. The

detailed nature of the charge order appear to be highly nonuniversal, and certainly cannot be used as a diagnostic tool for theories of pseudogap.

4 Neutron scattering

4.1 Unpolarized neutron scattering

For unpolarized neutron scattering, the differential scattering cross sections for Bragg scattering from an ordered array of orbital currents is given by⁵

$$\left(\frac{d\sigma}{d\Omega}\right) \propto \frac{|\langle \mathbf{j}(\mathbf{q}) \rangle|^2}{q^2}, \quad (4)$$

where \mathbf{q} now is the momentum transfer. We certainly do not know the form factors $\alpha(\mathbf{q})$ and $\beta(\mathbf{q})$ beyond their limiting forms, but a reasonable guess can be made to see the robust features of the intensity modulation as a function of the momentum transfer. For this purpose, we have chosen $\alpha(\mathbf{q}) = f(q)e^{-(\frac{q_x}{q_0})^2}$, and $\beta(\mathbf{q}) = f(q)e^{-(\frac{q_z}{q_1})^2}$. So, the intensity is parametrized by a orthorhombicity parameter $\lambda(\mathbf{q}) = e^{-[(\frac{q_x}{q_0})^2 - (\frac{q_z}{q_1})^2]}$ and $\beta(\mathbf{q})$. Note that all other factors, such as the magnitude of the order parameter, drop out if we normalize with respect to a reference Bragg reflection intensity. We then replace $\beta(\mathbf{q})$ by the well known Cu form factor,¹¹ which is likely to be an upper bound because the orbital currents are more spread out in real space than atomic orbitals. We choose $q_0 = 2\pi/d$ and $q_1 = 0.275q_0$. We shall see that the unpolarized intensity is not sensitive to the choice of the λ -parameter.

There is no question that the unpolarized neutron scattering intensities are dramatically different for orbital currents in comparison to spins lying in the a - b plane as shown in Fig. 2. The scattering from spins pointing along the c -direction can be easily calculated and is similar to the scattering from orbital currents. These two cases can be distinguished by going to higher order Bragg reflections such (H, H, L) , for $H > 1/2$, for example $(3/2, 3/2, L)$. The results for orbital currents fall off very rapidly in contrast to spins pointing in the c -direction.

4.2 Polarized neutron scattering

The Bragg scattering intensity for polarized neutrons from orbital currents is given by

$$\left(\frac{d\sigma}{d\Omega}\right)_{i \rightarrow f} \propto \frac{1}{q^4} |\langle f | \vec{\mu} | i \rangle \cdot \mathbf{q} \times \langle \mathbf{j}(\mathbf{q}) \rangle|^2, \quad (5)$$

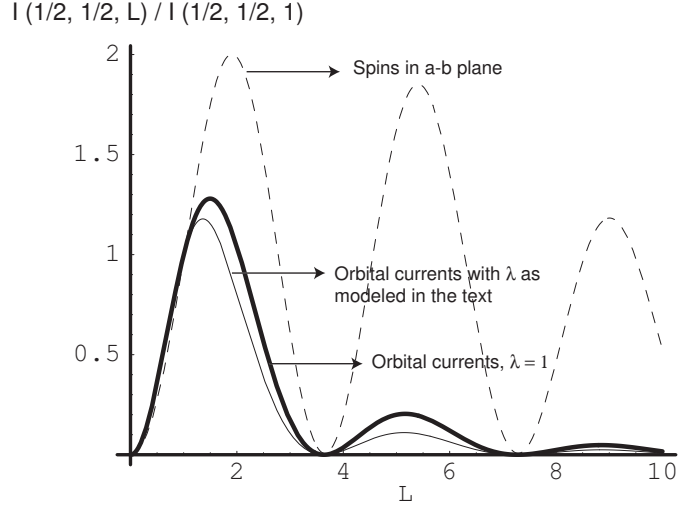


Figure 2. Normalized intensity, I , of Bragg reflections as a function of the perpendicular momentum transfer, q_z . The shorthand notation is $I(H, K, L) \equiv I(2\pi H/a, 2\pi K/a, 2\pi L/c)$. The intensity from spins lying in the a - b plane is obtained from the form factor given in Ref. 11.

where $\vec{\mu}$ is the neutron spin, and $|i\rangle$ and $|f\rangle$ are the initial and the final states of the neutron. It is easy to see that if the scattering vector is parallel to the direction of polarization, the entire scattering is spin flip. This is useful to identify magnetic scattering from non-magnetic scattering and the intensity ratios should follow the same pattern as that of the unpolarized case. When the scattering vector \mathbf{q} is perpendicular to the polarization, there can be both spin-flip and non-spin-flip scattering. This geometry contains additional information, which is the ratio of the spin-flip to non-spin-flip scattering. A common experimental set up is to polarize neutron along along the $[1, \bar{1}, 0]$ direction as shown in Fig. 3, so that the new x -axis is along $[1, 1, 0]$, and the new y -axis is along $[0, 0, 1]$.

Then a simple calculation shows that the ratio of the non-spin-flip to spin-flip scattering intensity, NSF/SF , for Bragg reflection (H, H, L) is

$$\frac{NSF}{SF} = 2 \left(\frac{\lambda(L) - 1}{\lambda(L) + 1} \right)^2 \left(\frac{Hc}{La} \right)^2 \left[1 + \frac{1}{2} \left(\frac{La}{Hc} \right)^2 \right], \quad (6)$$

which vanishes identically if there is no orthorhombicity, that is, $\lambda(L) = 1$.

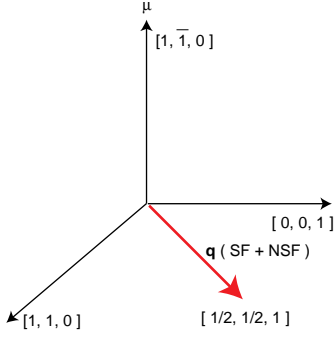


Figure 3. The vertical field geometry.

This is a nontrivial result for orbital current theory.

For the choice of the parameters described earlier, corresponding to $\lambda(L = 1) \approx 0.4$, this ratio for the reflection $(1/2, 1/2, 1)$ turns out to be ≈ 1 . Thus, while modeling of the orthorhombicity of the current distribution had very little effect on the unpolarized intensity, its effect on the polarized scattering is striking, turning the ratio (NSF/SF) to order 1 as compared to 0.

5 Concluding remarks

Other possible evidence against spin order is the existence of a spin gap due to the Ising universality class of the DDW order, and the small moment of order $2 \times 10^{-2} \mu_B$ corresponding to the field due to circulating currents. We made an educated guess for the microscopic nature of the current distribution. Clearly, we need a better understanding of it, although the ratio of the intensities as a function of the momentum transfer for unpolarized scattering is very insensitive to the modeling of the current distribution. Thus, we believe that our results are quite robust.

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